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SECOND-ORDER CLOSURE OF TURBULENT REACTING SHEAR FLOWS

by
Ashok K. Varma

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Aeronautical Research Associates of Princeton, Inc.
50 Washington Road, Princeton, New Jersey 08540
(609)-452-2950

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A second-order closure program for turbulent, compressible, reacting shear flows has been developed by A.R.A.P. The program is being extended to handle multi-component, multi-step chemical reactions, and will be used to study the mixing region of HF and DF chemical lasers.

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SUMMARY

For a number of turbulent flow problems, a first-order closure or eddy transport approach to the modeling of the turbulence is not sufficiently accurate. It is necessary that a more powerful approach be used to study the dynamics of the turbulence. Flows involving chemical reactions, such as those in a chemical laser, are good examples of flows requiring a more powerful approach. The mixing in HF and DF chemical lasers takes place under conditions of very large heat release. The coupling between the heat release and the turbulence is an important feature of the flow. A.R.A.P. has been funded under AFOSR Contracts F44620-73-C-0027 and F44620-75-C-0026 to employ this basic method to investigate problems connected with chemical lasers of particular interest to the Air Force Weapons Laboratory. These studies have resulted in considerable insight into the complex processes occurring in laser cavities. These studies have been documented in References 1, 2, and 3.

This progress report describes recent results of studies using the reacting shear layer (RSL) computer program and discusses the proposed procedure for handling multi-step chemical reactions in a second-order closure computation of turbulent reacting flows.

I. INTRODUCTION

A second-order closure program for the investigation of turbulent, compressible, chemically reacting flowfields is under development at A.R.A.P. Second-order closure methods have provided an understanding of the physics of turbulent flows which could not be provided by classical first-order closure techniques such as the eddy viscosity method. We have successfully applied these techniques to a variety of turbulent flow problems including incompressible and compressible shear layers,[2] the behavior of the planetary boundary layers,[4] and the dispersal of chemically reacting pollutants in a turbulent atmosphere.[5]

A.R.A.P. is funded under AFOSR Contract No. F44620-75-C-0026 to develop an invariant second-order closure model capable of investigating the mixing and reactions in HF and DF chemical lasers. The mixing in these devices takes place under conditions of large local heat release due to the highly exothermic chemical reaction. The interaction between the heat release and the turbulence is an important feature of the flow.

The set of second-order closure equations governing the mixing and reaction of compressible, turbulent, multi-component reacting shear layers has been modeled and programmed for solution in our RSL program. This interim scientific report describes some recent results of studies using this program and discusses the proposed procedure for extending the program for studying multi-step chemical reactions in a second-order closure computation.

II. REACTING SHEAR LAYER (RSL) PROGRAM

The reacting shear layer program has been completely checked out over the past six months. Program predictions for nonreacting flows[6,7] (two-dimensional wake, heated wake, heated planar jet) are in good agreement with experimental measurements. Comparison of program predictions with experimental data for reacting flows is now underway. The RSL program has been used for computations of the HF chemical laser flowfield, hydrogen-air premixed combustion and diffusion flames and propane-air premixed combustion and diffusion flames. The calculations have been performed using two different models for the scalar correlations. One model (used during the model development stage) was to set all third-order (and higher-order) scalar correlations to zero. The other model is the A.R.A.P. "typical eddy" box model. Preliminary results for exothermic reacting flows[7] suggest that there is only a small difference between the calculations using these two models. More extensive tests are necessary to check the validity of this result for different flow geometries and in different flowfield regions. It is, of course, obvious that if the model involving setting the higher-order correlations to zero can be used for most of the calculations, it will lead to considerable program simplification and increase in speed.

The use of the "typical eddy" box model in these calculations has verified the basic concept of modeling the scalar correlations using a probability density function composed of a set of Dirac functions of variable strengths and position in the scalar phase space. The computations have also allowed us to determine some shortcomings of the present model. A number of simple modifications have already been made to the model to extend its applicability to more severe environments, and some other changes are currently under study.

The current version of the program is restricted to one-step forward reactions. In the past month, we have developed a procedure for handling multi-step reaction systems including the complete turbulence-chemistry interaction. The procedure is briefly described in the next section.

III. SECOND-ORDER CLOSURE FOR MULTI-STEP REACTION SYSTEMS

The "typical eddy" box model has been most extensively used up to now with three species (α, β and γ) flowfields. In principle, the model is quite general and can be extended to a large number of species. However, the direct addition of each new species in the second-order closure system will add ten equations for the means and second-order correlations and does not appear to be a reasonable procedure for complex reaction systems. Actually, such a procedure is not necessary.

Consider the mixing and reaction of two initially separate streams α and β. These streams can be known mixtures of a large number of chemical species. The streams mix and react following a large number of elementary reactions and form a mixture of product species designated as γ. We assume that:

1. The composition of mixtures α and β is fixed for the entire flowfield. There are no internal reactions among the species in these two reactant mixtures.

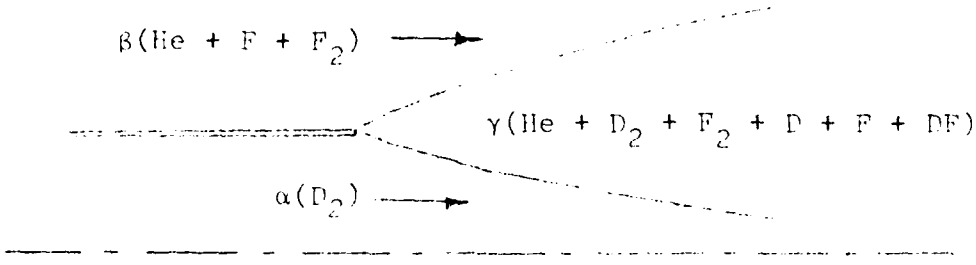
2. All the product species that compose γ are molecularly mixed. There are internal reactions within the γ species mixture. Due to the different rates of the various elementary reactions (between species present in α and β mixtures and the species present in γ), the composition of the mixture γ varies at different points across the flowfield.

Consider the following two-reaction system as an illustration of the procedure. The complete set of reactions that we will be using in our study of the DF chemical laser is presented in Table I.

$$D_2 + F \xrightarrow{k_1} DF + D$$

$$F_2 + D \xrightarrow{k_2} DF + F$$

α	D_2	known
β	$He + F + F_2$	known proportions
γ	$He + D_2 + F_2 + D + F + DF$	



The interaction between turbulence and chemistry only has to be taken into account for reactions between α and β, α and γ, and β and γ. Species within γ are assumed to be molecularly mixed and, therefore, species correlations do not have to be considered for the internal reactions. For convenience, we rewrite the reaction system as given below, tagging each chemical species with the mixture that it is a part of:

$$D_2(\alpha) + F(\beta) \rightarrow DF(\gamma) + D(\gamma)$$

$$D_2(\alpha) + F(\gamma) \rightarrow DF(\gamma) + D(\gamma)$$

$$D_2(\gamma) + F(\beta) \rightarrow DF(\gamma) + D(\gamma)$$

$$D_2(\gamma) + F(\gamma) \rightarrow DF(\gamma) + D(\gamma) \quad \text{internal reaction}$$

$$F_2(\beta) + D(\gamma) \rightarrow DF(\gamma) + F(\gamma)$$

$$F_2(\gamma) + D(\gamma) \rightarrow DF(\gamma) + F(\gamma) \quad \text{internal reaction}$$

We can now write the chemical source terms for the component species. For example,

$$\frac{d\overline{D_2}(\alpha)}{dt} = -k_1\left[\overline{D_2}(\alpha)\overline{F}(\beta) + \overline{D_2'(\alpha)F'(\beta)}\right] - k_1\left[\overline{D_2}(\alpha)\overline{F}(\gamma) + \overline{D_2'(\alpha)F'(\gamma)}\right]$$

$$\frac{d\overline{D_2}(\gamma)}{dt} = -k_1\left[\overline{D_2}(\gamma)\overline{F}(\beta) + \overline{D_2'(\gamma)F'(\beta)}\right] - k_1\left[\overline{D_2}(\gamma)\overline{F}(\gamma)\right] \quad , \text{ etc.}$$

Two other pieces of information are now required to complete this formulation. First, we will be solving equations for the second-order correlations $\overline{\alpha'\beta'}$, $\overline{\alpha'\gamma'}$, and $\overline{\beta'\gamma'}$. Now, $\overline{D_2'(\alpha)F'(\beta)}$, $\overline{D_2'(\alpha)F'(\gamma)}$, etc., can be simply calculated from these correlations when one knows the composition of the mixtures, and so the source terms are completely determined. Second, we have to find the total loss of $\bar{\alpha}$ and $\bar{\beta}$. In the above example, β is being lost due to the consumption of both $F(\beta)$ and $F_2(\beta)$. We determine the term that causes the greater loss of β and use the figure. If at some point the consumption of $F(\beta)$ leads to the larger loss of β, then one has to keep track of the corresponding components $F_2(\beta)$ and $He(\beta)$ that now become part of γ. The composition of γ has to be calculated at each point across the flowfield.

This procedure operates within the framework of three overall species mixtures α, β, and γ and the models and equations

developed earlier can still be used. The only change required is in the solution of the mean chemical species wherein we consider the complete set of elementary reactions. At the present time, we are making the program changes to study the DF chemical laser flowfield using all the elementary reactions listed in Table I.

IV. CONCLUSIONS

A computer program for a second-order closure computation of turbulent, compressible, reacting shear layers has been developed at A.R.A.P. The program has been tested for a variety of nonreacting and reacting flowfields and good results have been obtained. The program is currently being extended to handle multi-step multi-species chemical reactions.

TABLE I

	Reactions Being Considered							KF=A*EXP(P/RT)/T**N (MOLEC-KL-SEC UNITS)		
								A	N	E
1	F	+	D2	=	DF1	+	D	0.1929E 16	0.9	-2000.0
2	F	+	D2	=	DF2	+	D	0.4582E 16	0.9	-2000.0
3	F	+	D2	=	DF3	+	D	0.7235E 16	0.9	-2000.0
4	F	+	D2	=	DF4	+	D	0.9888E 16	0.9	-2000.0
5	DF1	+	DF0	=	DF0	+	DF0	0.1025E 03	-2.9	3200.0
6	DF2	+	DF0	=	DF1	+	DF0	0.1989E 03	-2.9	3200.0
7	DF3	+	DF0	=	DF2	+	DF0	0.3015E 03	-2.9	3200.0
8	DF4	+	DF0	=	DF3	+	DF0	0.4040E 03	-2.9	3200.0
9	DF1	+	D2	=	DF0	+	D2	0.5607E 02	-3.0	0.0
10	DF2	+	D2	=	DF1	+	D2	0.1145E 03	-3.0	0.0
11	DF3	+	D2	=	DF2	+	D2	0.1688E 03	-3.0	0.0
12	DF4	+	D2	=	DF3	+	D2	0.2231E 03	-3.0	0.0
13	DF1	+	F	=	DF0	+	F	0.2834E 16	0.7	-3600.0
14	DF2	+	F	=	DF1	+	F	0.3316E 16	0.7	-3600.0
15	DF3	+	F	=	DF2	+	F	0.4462E 16	0.7	-3600.0
16	DF4	+	F	=	DF3	+	F	0.8441E 15	0.7	-3600.0

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